

HOW TO

Use the New Features



SciFinder®

March 2010

SciFinder® offers many new structure drawing, reaction search and display, answer set manipulation, and results post-processing features and enhancements. Improved performance combined with improved integration with your work further enhances your overall SciFinder experience.

Structure Drawing

Keyboard Shortcuts and Paste from ChemDraw

1. The structure editor Pencil Tool now includes keyboard shortcut functions to quickly highlight, and with a simple keystroke, change an atom or bond in a structure drawing. (Click on the Shortcut Keys hyperlink to open this feature)
2. Clickable bonds make it easy to change bond types (single-double-triple) or easily sprout bonds from a carbon atom.
3. SciFinder now provides the ability to paste structures generated by ChemDraw into the structure editor.

The screenshot shows the 'Structure editor - LTDemo.mol' window. The main canvas displays a chemical structure consisting of a central six-membered ring connected to a five-membered ring on the left and another six-membered ring on the right. A toolbar on the left contains various drawing tools. A 'Shortcut Keys' dialog box is open on the right, listing elements and bonds with their corresponding keyboard shortcuts. The dialog box has a pink border. Below the dialog box, there are options for 'Drawing Editor' (Structure and Reaction) and 'Get substances that match your query using:' (Exact search, Substructure search, Similarity search). At the bottom, there are 'OK' and 'Cancel' buttons.

Elements/Shortcuts	Keyboard Shortcuts
a	A
A	ak
b	Br
B	Cb
c	C
C or I	Cl
e	Et
f	F
h	H
H	Hy
i	I
k	K
m	M
n	N
N	Na
o	O
P	P
P or 4	Ph
q	Q
s	S
S	Si
x	X
y	Cy
1	Bu-n
2	Bu-s
3	Bu-t

Bonds	Single	Double	Triple
1			
2			
3			

Reaction Search and Display

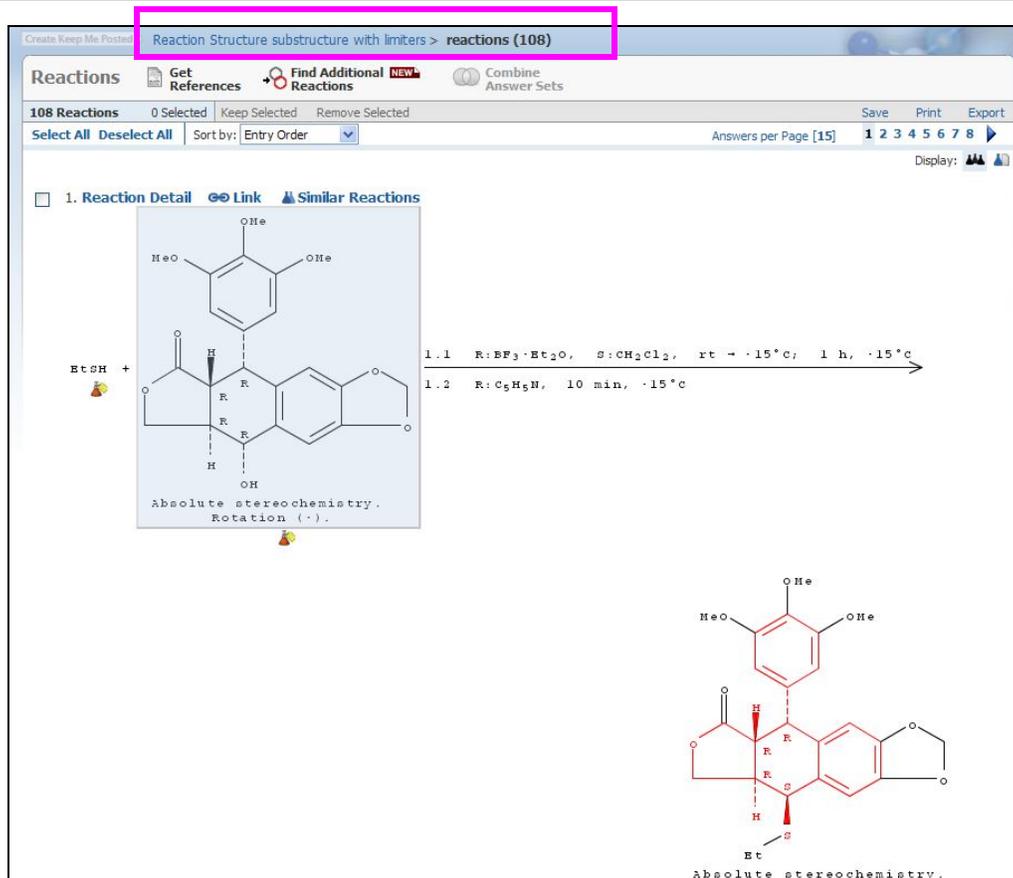
Non-participating Functional Groups

1. A Non-participating Functional group is a functional group in a reactant that is mapped to the same functional group in a product and which survives the reaction unchanged.
2. Non-participating Functional Groups can be used to Limit or Refine an answer set to reactions that include one or more functional groups and/or functional group classes in a non-participating role.
3. Draw a reaction query, then select one or more Non-participating Functional Groups from the list.

The screenshot displays the 'Explore Reactions' interface. At the top, it shows the breadcrumb 'Reaction Structure substructure > reactions (122)'. Below this, there are two tabs labeled 'Reaction Structure'. A chemical structure is shown in the center, with a caption 'Click image to change structure or view detail'. Below the structure, there are search type options: 'Allow variability only as specified' (selected) and 'Substructure'. A 'Solvent(s)' section is visible, with a 'Select Solvents' button. A 'Non-participating Functional Group(s)' dropdown menu is highlighted with a pink box. Below it, a 'Close' button with a 'NEW' tag is visible. A 'View:' dropdown is set to 'All' with '217' items. A list of functional groups is shown, with 'Lactone' selected and highlighted by a pink box. The list includes: Ketenimine, KETONES, Lactam, Lactone, Mesyl, Metal Arene, Metal Carbene, Metal Carbonyl, Metal Cyclopentadienyl, Metal Halide, and Metal Hydride. At the bottom, there are radio buttons for 'all selections' (selected) and 'any selection'.

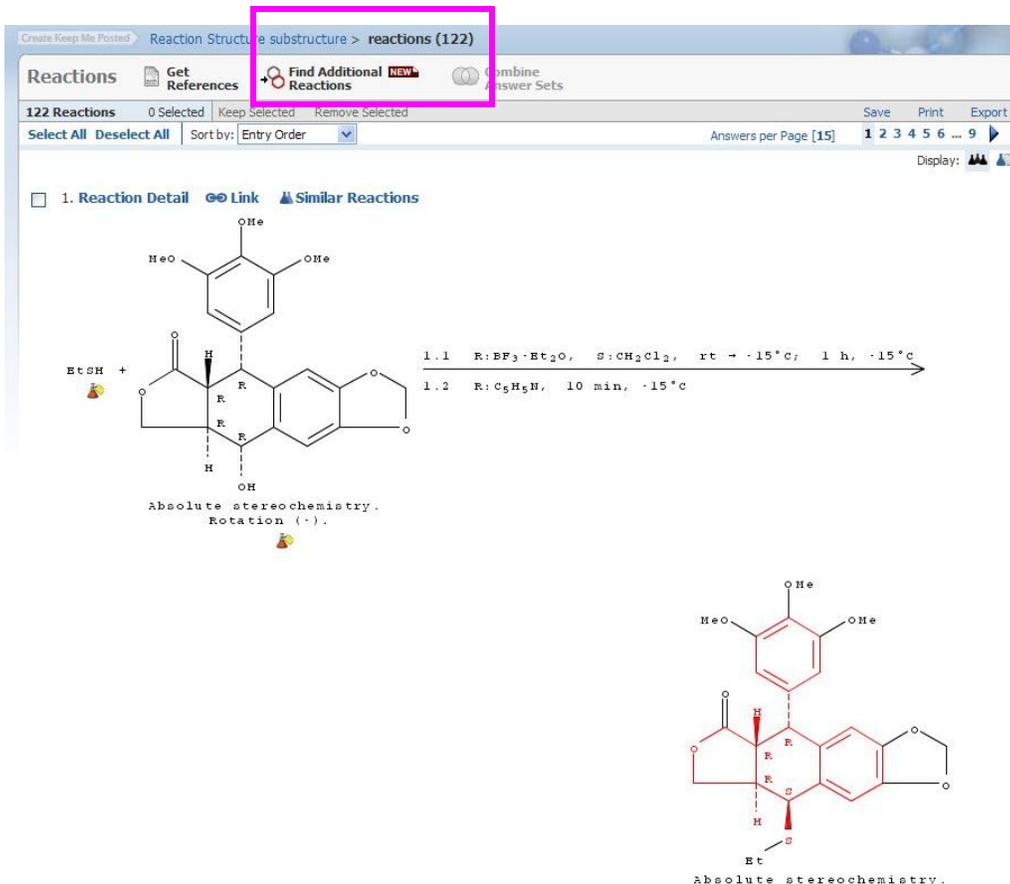
Non-participating Functional Groups (cont.)

4. After running the reaction substructure search with the lactone non-participating functional group limiter, the results are more targeted to reactant and product structural characteristics.



Find Additional Reactions

1. **Find Additional Reactions** searches references that contain structurally matching substances that have a synthetic preparations role.
2. Select **Find Additional Reactions** to search for reactions matching the reaction answer set query. Note the original query resulted in 122 reactions.



Find Additional Reactions (cont.)

- The new answer set of 295 reactions contains 187 Additional Reactions. There are no reaction conditions or reactants.

The display shows a product and the number of references associated with it.

The screenshot shows a web interface for finding additional reactions. At the top, it says "Reaction Structure substructure with limiters > reactions (108) > find additional reactions (295)". Below this, there are tabs for "Reactions", "Get References", and "Combine Answer Sets". The "Reactions" tab is active, showing "295 Reactions" and "187 reactions with the Answer Types Additional Reactions are displayed". There are buttons for "Select All", "Deselect All", and "Sort by: Entry Order". On the right, there is an "Analysis" panel with a dropdown for "Analyze by:" set to "Answer Type". Below this, it says "Click bar to view only those reactions within the current answer set" and shows a bar chart for "Additional Reactions" with a value of 187. There is a "Show More" button. In the main area, there is a "Reaction Detail" section for reaction 109, showing a chemical structure of a complex molecule with a benzene ring substituted with two methoxy groups and a furan ring. Below the structure, it says "1 reference".

Enhanced Reaction Display – Commercial Sources

- Reaction display now contains icons to indicate commercial source availability.

Click the commercial source icon to see supplier information.

The screenshot shows an enhanced reaction display. At the top, it says "Reaction Structure substructure > reactions (122)". Below this, there are tabs for "Reactions", "Get References", "Find Additional Reactions", and "Combine Answer Sets". The "Reactions" tab is active, showing "122 Reactions" and "0 Selected". There are buttons for "Select All", "Deselect All", and "Sort by: Entry Order". On the right, there is an "Analysis" panel with a dropdown for "Analyze by:" set to "Catalyst". Below this, it says "Click bar to view only those reactions within the current answer set" and shows a bar chart for "Catalyst" with values: Et3N (9), (EtO)2P(=O)CN (4), and AcOH (3). There is a "Show More" button. In the main area, there is a "Reaction Detail" section for reaction 1, showing a chemical structure of a complex molecule with a benzene ring substituted with two methoxy groups and a furan ring. Below the structure, there are reaction conditions: "1.1 R: BF3 · Et2O, S: CH2Cl2, rt - -15 °C, 1 h, -15 °C" and "1.2 R: C5H5N, 10 min, -15 °C". Below the conditions, there is a "Commercial Source" icon (a small yellow icon with a magnifying glass) which is highlighted with a pink box. Below the icon, it says "Absolute stereochemistry." and "R". Below the structure, there is a "Commercial Source" icon (a small yellow icon with a magnifying glass) which is highlighted with a pink box. Below the icon, it says "Absolute stereochemistry." and "Rotation (-). 59%".

Designating Preferred Suppliers

Selecting a Supplier

1. Select a supplier to see additional Commercial Source Detail.

Reaction Structure substructure > reactions (122) > commercial sources (74) > ALDRICH

Commercial Sources

74 Commercial Sources 1 Selected Keep Selected Remove Selected Print Export

Select All Deselect All Sort by: Catalog Name Answers per Page [20] 1 2 3 4

- 1. **3B Scientific Corporation Product List**
Supplier Name: 3B Scientific Corporation, Catalog Publication Date: 1 Jan 2010
Order Number: 3B2-5384, Quantity: 5g
518-28-5 Podophyllotoxin
[Link](#)
- 2. **ABCR Product List**
Supplier Name: ABCR GmbH KG, Catalog Publication Date: 11 Apr 2007
Order Number: AB167899, Quantity: 25 mg
518-28-5 (-)-Podophyllotoxin
[Link](#)
- 3. **ACC Corp. Chemical Compounds Catalog**
Supplier Name: American Custom Chemicals Corp., Catalog Publication Date: 21 May 2009
Order Number: HBL0000185, Quantity: 100mg, 1g, 10g, 100g
518-28-5 Podophyllotoxin
[Link](#)
- 4. **Acros Organics**
Supplier Name: Thermo Fisher Scientific, Catalog Publication Date: 12 May 2008
Order Number: 22841, Quantity: 100mg
518-28-5 Podophyllotoxin
[Link](#)
- 5. **AK Scientific Product Catalog**
Supplier Name: AK Scientific, Inc, Catalog Publication Date: 1 Jan 2010
Order Number: 70719, Quantity: 100g, 1g, 25g, 5g
518-28-5 Podophyllotoxin
[Link](#)
- 6. **ALDRICH**
Supplier Name: Sigma-Aldrich, Catalog Publication Date: 1 Jan 2010
Order Number: 858447, Quantity: 1 g
518-28-5 Podophyllotoxin
[Link](#)

Designating Supplier Status

1. Clicking on **Status** provides the ability to designate a supplier as preferred or non-preferred. The default status is Unclassified.

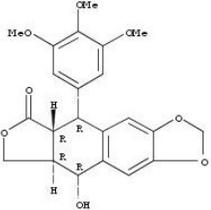
Reaction Structure substructure with limiters > reactions (108) > commercial sources (74) > ALDRICH

Commercial Source Detail

Link Print Export Previous Next

6. ALDRICH

Catalog Information Catalog Publication Date: 1 Jan 2010 Order Number: 858447 Quantity: 1 g, Price: contact supplier	Substance Information CAS Registry Number: 518-28-5 Podophyllotoxin
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Absolute stereochemistry. Rotation (-).

Catalog Suppliers

Below are the contributing supplier(s) to this catalog.

Supplier Name	Address	Contact Information	Status <small>NEW</small>
Sigma-Aldrich	P O Box 14508 St. Louis, MO 63178 USA	Phone: 1-800-325-3010 Phone: 1-314-771-5765 Phone: 1-314-771-5750 (Call Collect) Fax: 1-800-325-5052 Fax: 1-314-771-5757 Web: http://www.sigma-aldrich.com Please see website for additional locations around the world.	Preferred Non Preferred Unclassified

View Preferred Suppliers in an answer set

1. In subsequent displays of commercial sources your preferred suppliers are indicated.

The screenshot shows a web interface for 'Commercial Sources'. At the top, there are options for 'Print' and 'Export'. A yellow warning banner states: 'The chemical supplier information is provided on an "as is" basis. Please consult the suppliers for current information regarding pricing, regional availability, available quantities, purities, etc. THERE ARE NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. ACS is not liable for any loss of profit, goodwill or any other damages arising out of the use of this information.' Below this, there are controls for 'Select All', 'Deselect All', and a 'Sort by' dropdown menu set to 'Supplier Preference'. The main list contains four entries, each with a checkbox and a green checkmark icon. The text 'Catalog is associated with a preferred supplier(s)' is highlighted in a pink box for each entry. The entries are: 32. ALDRICH, 4. Fluka, 3. SJAL, and 79. SIGMA. To the right, an 'Analyze by:' sidebar shows a 'Supplier Preferences' dropdown and a list of suppliers with counts: SIGMA-ALDRICH, ST. LOUIS, USA (4); VWR INTERNATIONAL, LLC, WEST CHESTER, USA (4); Unclassified (74); and Non Preferred (1). A 'Show More' button is at the bottom of the sidebar.

Add/Edit Suppliers in Preferences

1. There is a new **My Suppliers** Preferences option that provides the capability to add/edit suppliers and maintain lists of those that are preferred and non-preferred.

The screenshot shows the 'My Suppliers' interface. At the top, there is a 'My Suppliers' header with an 'Add/Edit Suppliers' button highlighted in a pink box. Below the header, there is a 'Return to Preferences' link. The main content is divided into two sections: 'Preferred Suppliers (1)' and 'Non-Preferred Suppliers (0)'. The 'Preferred Suppliers' section contains a table with columns for 'Supplier Name', 'City', and 'Country'. The table has one row: AURORA FINE CHEMICALS LLC, SAN DIEGO, USA. A small 'x' icon is visible in the top right corner of the table. The 'Non-Preferred Suppliers' section is currently empty and contains a message: 'You currently have no Non Preferred suppliers. To add suppliers to a list, click Add/Edit Suppliers, then locate a supplier, and designate a preference.' A 'Return to Preferences' link is also present at the bottom right of this section.

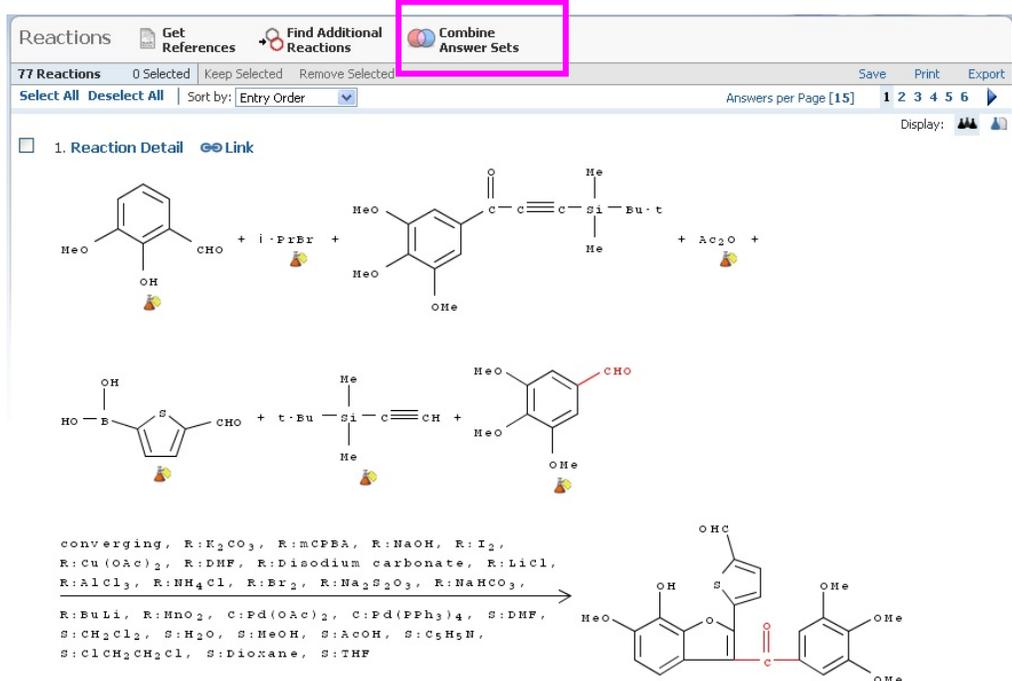
Usability Enhancements

Combine Current and Saved Answer Sets

1. SciFinder allows you to combine a current and 1 or more saved answer sets into a new answer set. Only entire answer sets can be combined. You cannot add selected answers from the current answer set to one or more saved answer sets.

2. To combine a current answer set and one or more saved answer sets first run a search that retrieves an answer set for References, Substances, or Reactions, and then click **Combine Answer Sets**.

3. The Combine Answer Sets dialog displays. It lists the current answer set and the saved answer sets of the same type.



Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (295):

3 Answer Sets 1 Selected	reaction Answer Set Details	Date Saved
<input type="checkbox"/>	quercetin as reactant (11551) Reaction Structure substructure > reactions (11551)	Jun 16, 2009
<input type="checkbox"/>	quercetin as product (2233) Reaction Structure substructure > reactions (2233)	Jun 16, 2009
<input checked="" type="checkbox"/>	caffeine reactions limited by water as a solvent (2162) Reaction Structure substructure with limiters > reactions (2162)	May 28, 2009

Select an option for combining the answer sets:

Combine Include all answers from both sets

Intersect Include only answers that appear in both sets

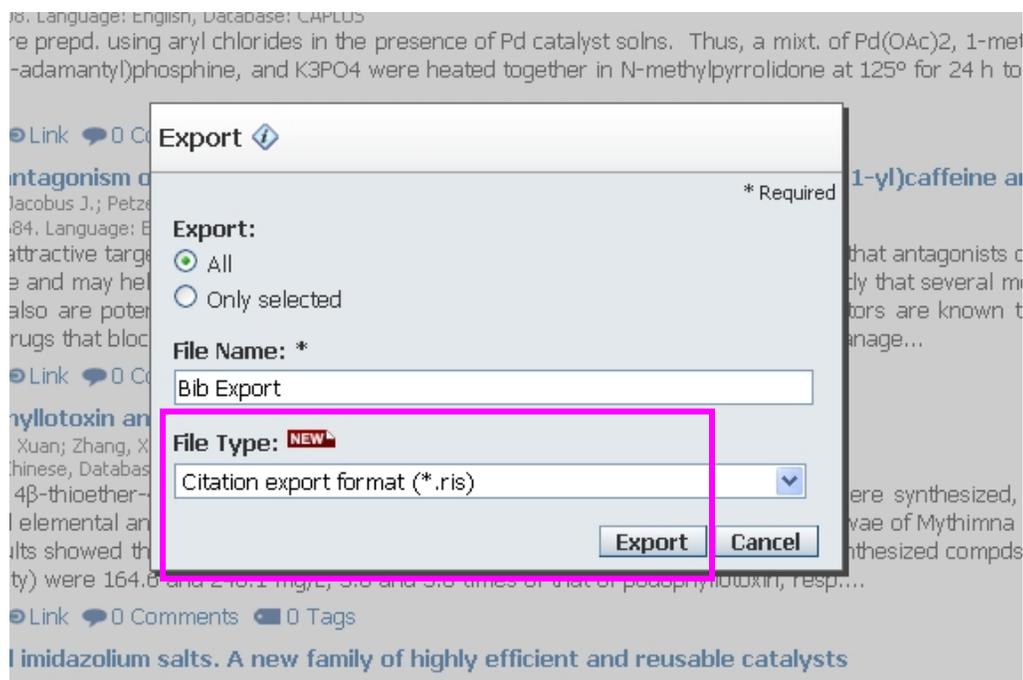
Exclude Include only answers from **Current answer set (295)** that are not in **caffeine reactions limited by water as a solvent (2162)**

Exclude Include only answers from **caffeine reactions limited by water as a solvent (2162)** that are not in **Current answer set (295)**

Combine Answer Sets Cancel

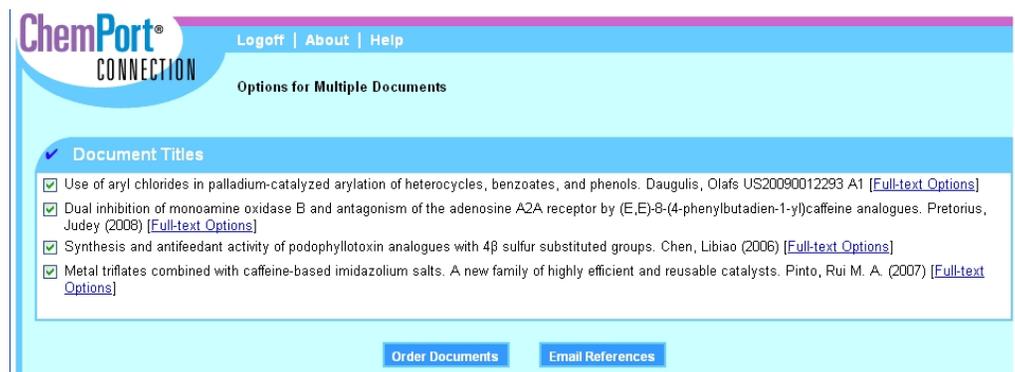
Export Answers in .ris Format

1. Use the Export function to save a copy of an answer set on your computer. Answers can be exported in several formats. New with this release is export to the .ris format, which allows SciFinder references to be imported into citation software, such as EndNote® and Reference Manager®.



Get Full Text for multiple documents

1. You can now make multiple fulltext document requests at one time.



.sfr to .akx File Conversion Tool

1. CAS now provides a free tool for converting client based saved answer set (.sfr) files to the new, web-based .akx format.

The tool is available at:

<https://scifinder.cas.org/utills/sfr2akx/>

SciFinder® sfr to akx Conversion Tool

File Selection

Username

Filename

Your SciFinder username is assigned to you alone and may not be shared with anyone else.

sfr to akx Conversion Tool

Follow these steps to convert SciFinder client files (.sfr) to the new web format (.akx).

1. In the File Selection box enter your Username.
2. Click the Browse button to locate and select the .sfr file or .zip collection of multiple .sfr files you wish to convert.
3. After you have finished making your selection click the "Convert to akx" button
4. After the conversion to akx format has completed you will be prompted to either Save the resulting .akx file (or .zip file containing multiple .akx files) or choose a program to Open it. **Select the Save option.**
5. If problems are encountered in the conversion process, you will receive either, an on-screen alert in the case of a single .sfr file conversion, or a .zip file containing a Readme file with details of successful or failed conversions if a .zip collection was used originally. The conversion tool will ask you to save or open this file.
6. To import the .akx file into SciFinder, login and then click the Import button which is located in the Saved Answer Sets area on the right side of any Explore page. When the Import Answer Set dialog box appears, click Browse to locate the .akx file you wish to import and then click OK to import the file.

Note: .zip is the only compression format supported by this tool. (More information on working with .zip files.)

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